

Book Reviews

Data analysis for chemists, David Livingstone, Oxford Science Publications, Oxford University Press, UK, 1995, xvi + 239 pp., price UK£40.00. ISBN 0-19-855728-0

The subtitle to this book, 'Applications to QSAR and Chemical Product Design', gives a better indication of its contents. Professor Livingstone is a leading authority in this research area, having formerly managed the QSAR section at SmithKline Beecham Pharmaceuticals and having made a number of seminal contributions to advance the research in this field. The book is a successful practical account of how to do QSAR, particularly, but not entirely, with respect to medicinal chemistry. In my estimation, the book deserves to be on the desk of all scientists and students working with QSAR methods.

In some chapters, the book uses boxing devices for supplementary material which need not be read by an informed student but would be very useful for a newcomer. The book is based on the need for a fair knowledge of statistics and leads the reader through a number of examples, with sufficient tables of data and figures, to allow a good appreciation of the problem. My guess is that students who have read this book carefully will not encounter much difficulty when putting the methods into practice. The author is at pains to point out the many pitfalls that may plague an unthinking application to molecular design.

Chapter 1 begins with the concept that various molecular properties can be quantified as molecular parameters, and that these parameters may be related to the activity within a series of compounds. The fundamental problems which face the practitioner of QSAR are centred on a proper experimental design. In the past, many QSARs have subsequently been found to be flawed because the statistical design was inadequate. Chapter 2 will remind readers of the constant need for vigilance against weak experimental design; students would be well advised to discuss these problems in tutorials. The need for transforming data into a standardised form is covered in chapter 3 where the problem of multicollinearity is highlighted. Chapter 4 emphasises the need to examine the data by certain display methods. Pictures of data patterns give the user an intuitive feel for relationships, whether data show clustering, perturbation by outliers and other odd sta-

tistical quirks which can easily be missed if not inspected. In chapter 5 we are treated to a discussion of topics grouped as Unsupervised Learning; factor analysis and cluster analysis are handled well and significance for clusters is explained. Regression analysis, often a topic which students find difficult for multiple regression problems, is dealt with painlessly. In my opinion chapter 6 is probably the best 25 pages that can be found on the subject. Discriminant analysis and partial least squares form the content of chapter 7. Multivariate analysis is described in chapter 8 and covers principal components and factor analysis, cluster analysis, spectral-map analysis and models for dependent and independent data. The last chapter delves into new methods of artificial intelligence applied to data analysis. An area in which the author has been pre-eminent is the application of neural networks to deriving functional relationships between structure and activity. Perhaps modesty has restricted the length of this section; I would have preferred a little more, owing to my optimism about that area of research.

I am very positive about the value of this book. It is impeccably written and will be my choice to recommend to students learning about QSAR.

P. M. Dean

ACS Symposium series 582

Allelopathy: organisms, processes, and applications, ed. Inderjit, K. M. M. Dakshini & F. A. Einhellig, American Chemical Society, Washington DC, 1995, x + 381 pp., price US\$99.95. ISBN 0 8412 3061 7

In its simplest sense, allelopathy may be defined as the release of a chemical by one plant or micro-organism that inhibits the growth of nearby plants or micro-organisms and so reduces competition for space and resources for growth. More recently it is regarded as a complex of subtle chemical communications that encompass the interactions of micro-organisms, insects and higher animals with the plant kingdom in natural or agricultural ecosystems.

We are now certain that micro-organisms and plants release volatile organic compounds from their surfaces and leachates from leaves and roots, and other allelochemicals are released into the environment on their

death and decomposition. The agents themselves are invariably secondary metabolites arising from the shikimate or acetate/mevalonate pathways, including a vast array of phenols and phenylpropanes, acetogenins, terpenoids, steroids and alkaloids. However, many interactions remain poorly understood because they are interwoven with the complexities of plant growth in an ever-changing environment. Our challenge is to explain how allelochemicals act, but this is always complicated by chemical and biological diversity and interactions with stress phenomena, such as the prevailing growth conditions of temperature and the availability of light, water, space, nutrients and disease. Further complexity arises with the realisation that allelochemical inhibitions may result from the combined effects of several compounds of the same or different chemical class, and that phytotoxicity may result from action at many cellular sites rather than one discrete mode of action. Therefore, to unravel the precise details of allelopathic interactions is a formidable task and a major academic and commercial challenge.

This book provides, in 25 chapters, a collection of recent findings in allelopathy from leaders in the field, especially in agroecosystems, and is an important and thought-provoking account of the subject. After a well balanced overview, chapters 2 to 6 consider interactions with specific organisms, followed by six chapters dealing with proposed mechanisms of action. Chapters 13 to 18 focus on allelopathy in agroecosystems and the final seven chapters present opportunities for biocontrol and the possible applications of allelochemistry to the agrochemical industry. Each chapter is clearly presented and fully referenced, and the editors have produced the volume to a high standard.

Certain common points do emerge from the volume, perhaps the main one being that agricultural productivity and yield are routinely influenced by allelopathy. Utilising allelopathy may therefore aid modern agriculture. For example, novel crop rotations may be developed to capitalise on allelopathic activity in combination with herbicide use for weed control. Furthermore, allelochemicals are a readily available source of novel chemicals with biological activity towards plants. Their potential for exploitation as leads for herbicide development remains enormous.

There is something in this volume for all disciplines that contribute to Pesticide Science, from secondary product chemistry to biological control, and it can be recommended as providing an excellent background text to an important yet complex topic.

A. H. Cobb

American Chemical Society, Washington DC, 1994, x + 317 pp., price US\$79.95.
ISBN 0 8412 2923 6

A major advance in pesticide chemistry in recent years has been the development of new and potent molecules that act through the photodynamic action of porphyrins. All the major agrochemical companies own patents in this area and have dedicated laboratories and personnel to exploit their agrochemical potential. Initial commercial success with herbicides has more recently generated further lines of interest in the development of porphyrinic insecticides and the use of porphyrins as chemotherapeutic agents in humans, particularly in tumour therapy.

All organisms synthesize cycle tetrapyrroles which play central roles in life. Examples include the cytochromes in respiratory electron transport, the oxygen carrier haemoglobin and chlorophyll, the principal pigment in photosynthesis, to name but a few. Chemicals that inhibit the biosynthesis of tetrapyrroles lead to the accumulation of intermediates that are termed photodynamic compounds, which, in the presence of light and molecular oxygen, will generate highly reactive oxygen species, especially singlet oxygen. These free radicals are toxic to all living things since singlet oxygen is highly reactive to membrane lipids causing their photoperoxidation and hence membrane breakdown. A major and successful class of herbicides that includes the nitrodiphenyl ethers, oxadiazoles and *N*-phenylimides inhibit the enzyme protoporphyrinogen oxidase, the last common enzyme to both haem and chlorophyll biosynthesis, leading to the accumulation of the photodynamic intermediate protoporphyrinogen IX. The singlet oxygen attack in this case selectively kills weeds and the lack of chlorophyll in treated plants is clearly evident.

Fourteen of the 21 chapters of this book consider the porphyrinic pesticides as herbicides in great detail, covering their synthesis, chemical groups, structure-activity relationships, characterisation in plants and mode of action. The remaining seven chapters examine the use of photodynamic porphyrins as insecticides and pharmaceuticals, and include details of their mammalian toxicology and potential for use in cancer therapy.

The editors deserve praise both for their contributions to this field and for producing an excellent text. Its novelty and greatest value is that it brings together the findings of a very diverse group of scientists involved in several aspects of porphyrin research. Each chapter is well presented and referenced, and a wealth of relevant information is included. This book is a valuable source for all workers in the field and in particular pesticide scientists.

A. H. Cobb

ACS Symposium series 559

Porphyrinic pesticides: Chemistry, toxicology and pharmaceutical applications, ed. S. O. Duke & C. A. Rebeiz,